Mathematical Modeling

The reactions below shows the four-step reaction network for the conversion of methylmercury to volatile mercury using the mer operon in E. coli. This network involves the transport of methylmercury into the cell, its subsequent conversion into ionic and volatile mercury, and the transport of volatile mercury to the extracellular space. This simplified network follows the proposed mechanism of the mer operon and it captures the primary steps of methylmercury breakdown in E. coli.

$$CH_3Hg^+(ex) \rightarrow CH_3Hg^+(cyt)*$$

$$CH_3Hg^+(cyt) + MerB \rightarrow Hg^{2+}_{(cyt)} + MerB + CH_3^-$$

$$Hg^{2+}_{(cyt)} + MerA + 2NADPH \rightarrow Hg^0_{(cyt)} + MerA + 2NADP^+ + 2RSH$$

$$Hg^0_{(cyt)} \rightarrow Hg^0_{(ex)}$$

*According to research done by Mason et al., methylmercury diffuses into the cytosol.

Furthermore, a system of ordinary differential equations was used to model the biochemical reactions taken place at each step of the conversion process. The cofactors were not included in the equations because at sufficient concentrations, they do not significantly alter the rates.

$$\frac{dCH_3Hg^+(cyt)}{dt} = k_1 * [CH_3Hg^+(ex)]$$

$$\frac{dHg^{2+}(cyt)}{dt} = \frac{V_b*[CH_3Hg^+(cyt)]}{K_2+[CH_3Hg^+(cyt)]}$$

$$\frac{dHg^0(cyt)}{dt} = \frac{V_a*[Hg^{2+}]cyt}{K_3+[Hg^{2+}]_{cyt}+[Hg^{2+}]^2_{cyt}/K_4}$$

$$\frac{dHg^0(ex)}{dt} = k_5 * [Hg^0(cyt)]$$

k_1 = 100000 nM/hour
V_b =1830000 nM/hour K_2=1000 nM
V_a = 384000 nM/hour K_3=12600 nM K_4= 97600 nM
k_5=130992 nM/hour

The equations used in conversion steps 3 and 4 are extracted from studies done by Maria on ionic mercury uptake by *E. coli* cells (Maria, 2010). These equations can be used because ionic mercury is converted into elemental mercury which in turn diffuses into the extracellular space; these two steps were described in the Maria paper. It is assumed that methylmercury and ionic mercury have similar orders of magnitude of transport rate into the cell.